



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:11 pm GMT

PDB ID : 2XYJ
Title : NOVEL SULFONYLTHIA DIAZOLES WITH AN UNUSUAL BINDING MODE AS PARTIAL DUAL PEROXISOME PROLIFERATOR-ACTIVATED RECEPTOR (PPAR) GAMMA-DELTA AGONISTS WITH HIGH POTENCY AND IN-VIVO EFFICACY
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Deposited on : 2010-11-18
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

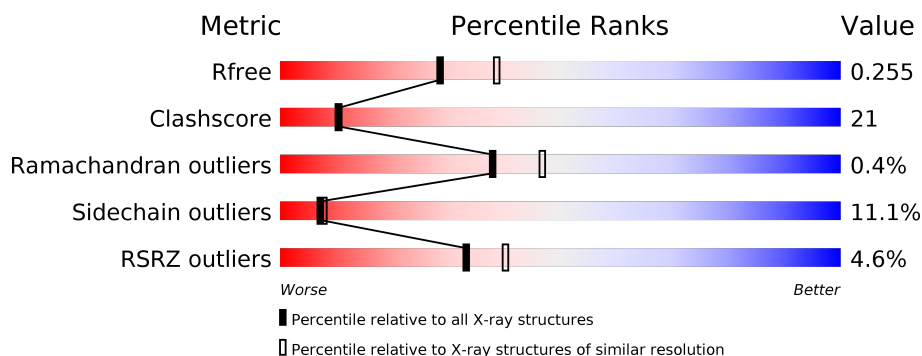
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	288	<div> <div>3%</div> <div>61%</div> <div>26%</div> <div>•</div> <div>9%</div> </div>
1	B	288	<div> <div>6%</div> <div>57%</div> <div>29%</div> <div>5%</div> <div>10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1PE	A	1443	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4450 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PEROXISOME PROLIFERATOR-ACTIVATED RECEPTOR DELTA.

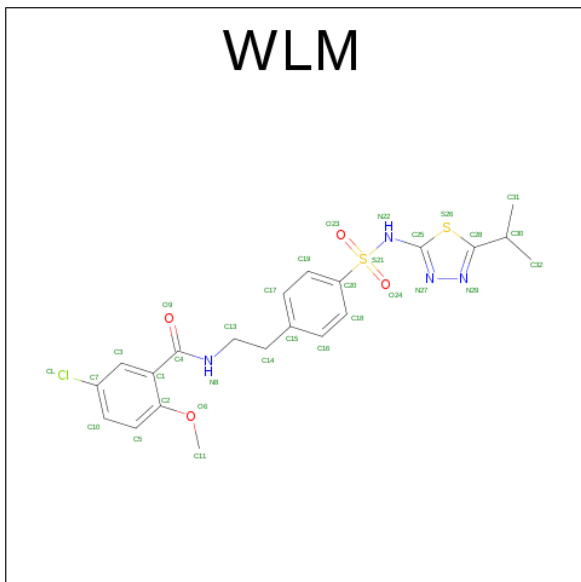
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2118	1371	357	380	10			
1	B	259	Total	C	N	O	S	0	0	0
			2084	1351	349	374	10			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	MET	-	EXPRESSION TAG	UNP Q03181
A	155	LYS	-	EXPRESSION TAG	UNP Q03181
A	156	LYS	-	EXPRESSION TAG	UNP Q03181
A	157	GLY	-	EXPRESSION TAG	UNP Q03181
A	158	HIS	-	EXPRESSION TAG	UNP Q03181
A	159	HIS	-	EXPRESSION TAG	UNP Q03181
A	160	HIS	-	EXPRESSION TAG	UNP Q03181
A	161	HIS	-	EXPRESSION TAG	UNP Q03181
A	162	HIS	-	EXPRESSION TAG	UNP Q03181
A	163	HIS	-	EXPRESSION TAG	UNP Q03181
A	164	GLY	-	EXPRESSION TAG	UNP Q03181
B	154	MET	-	EXPRESSION TAG	UNP Q03181
B	155	LYS	-	EXPRESSION TAG	UNP Q03181
B	156	LYS	-	EXPRESSION TAG	UNP Q03181
B	157	GLY	-	EXPRESSION TAG	UNP Q03181
B	158	HIS	-	EXPRESSION TAG	UNP Q03181
B	159	HIS	-	EXPRESSION TAG	UNP Q03181
B	160	HIS	-	EXPRESSION TAG	UNP Q03181
B	161	HIS	-	EXPRESSION TAG	UNP Q03181
B	162	HIS	-	EXPRESSION TAG	UNP Q03181
B	163	HIS	-	EXPRESSION TAG	UNP Q03181
B	164	GLY	-	EXPRESSION TAG	UNP Q03181

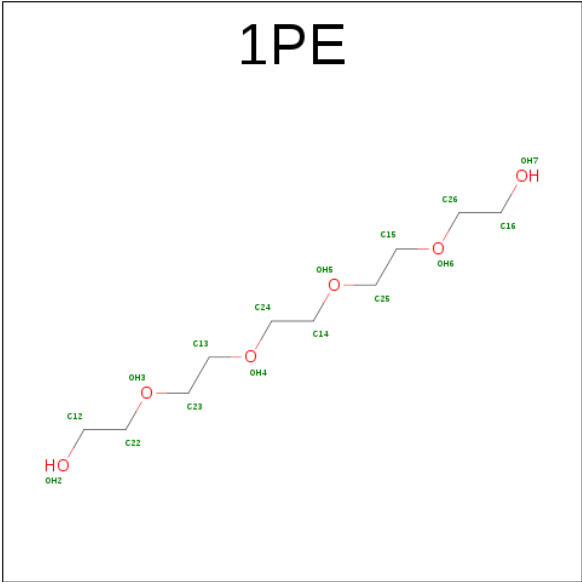
- Molecule 2 is 5-CHLORO-2-METHOXY-N-[2-[4-[(5-PROPAN-2-YL-1,3,4-THIADIAZOL-

2-YL)SULFAMOYL]PHENYL]ETHYL]BENZAMIDE (three-letter code: WLM) (formula: $C_{21}H_{23}ClN_4O_4S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 32	C 21	Cl 1	N 4	O 4	S 2	0	0
2	A	1	Total 32	C 21	Cl 1	N 4	O 4	S 2	0	0
2	B	1	Total 32	C 21	Cl 1	N 4	O 4	S 2	0	0
2	B	1	Total 32	C 21	Cl 1	N 4	O 4	S 2	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $\text{C}_{10}\text{H}_{22}\text{O}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	38	Total	O	0	0
			38	38		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	37.75Å 112.01Å 152.57Å 90.00° 95.71° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 37.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.30) 99.9 (37.55-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 2.29Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.208 , 0.250 0.211 , 0.255	Depositor DCC
R_{free} test set	2324 reflections (9.03%)	DCC
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4450	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: WLM, 1PE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/2163	0.60	0/2921
1	B	0.36	0/2128	0.55	0/2875
All	All	0.39	0/4291	0.58	0/5796

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2118	0	2155	99	0
1	B	2084	0	2122	79	0
2	A	64	0	46	7	0
2	B	64	0	46	7	0
3	A	16	0	22	16	0
4	A	66	0	0	3	0
4	B	38	0	0	2	0
All	All	4450	0	4391	181	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:GLU:HG3	2:A:1442:WLM:H142	1.20	1.19
1:A:435:GLU:CG	2:A:1442:WLM:H142	1.97	0.94
1:A:421:LYS:HZ2	1:A:434:GLN:HE21	1.12	0.91
1:A:421:LYS:NZ	1:A:434:GLN:HE21	1.68	0.90
1:A:365:MET:HE3	3:A:1443:1PE:H242	1.57	0.86
1:A:413:HIS:HA	1:A:416:MET:HE2	1.58	0.86
1:B:435:GLU:HG3	2:B:1442:WLM:H142	1.58	0.85
1:A:269:SER:HB3	1:A:373:ILE:CD1	2.08	0.83
1:A:283:LYS:HE3	1:A:439:ASP:HB2	1.61	0.82
1:A:365:MET:CE	3:A:1443:1PE:H242	2.11	0.81
1:B:264:ALA:HA	1:B:267:ILE:HD12	1.62	0.80
1:B:178:PHE:CE1	1:B:268:PRO:HG2	2.18	0.79
1:B:357:LEU:HD23	1:B:373:ILE:HB	1.64	0.79
3:A:1443:1PE:H221	1:B:236:PRO:HB3	1.64	0.78
1:A:435:GLU:HG3	2:A:1442:WLM:C14	2.08	0.78
1:B:413:HIS:HA	1:B:416:MET:HE2	1.66	0.78
1:A:216:ILE:HG13	4:A:2008:HOH:O	1.82	0.77
1:A:219:LEU:HD23	1:A:241:ILE:HD11	1.67	0.76
1:A:269:SER:HB3	1:A:373:ILE:HD13	1.69	0.75
1:A:423:THR:HG22	1:A:424:GLU:HG2	1.73	0.71
1:A:421:LYS:NZ	1:A:434:GLN:NE2	2.38	0.70
1:A:430:HIS:ND1	1:A:431:PRO:HD2	2.07	0.70
1:B:343:LEU:HD11	1:B:399:LEU:HD21	1.76	0.68
1:A:429:LEU:HB3	1:A:434:GLN:HG2	1.76	0.68
1:A:276:ASN:ND2	3:A:1443:1PE:OH5	2.27	0.68
1:A:430:HIS:CG	1:A:431:PRO:HD2	2.29	0.68
1:B:435:GLU:CG	2:B:1442:WLM:H142	2.23	0.68
1:B:314:ARG:NH2	1:B:329:GLU:OE2	2.27	0.67
1:A:268:PRO:O	1:A:269:SER:HB2	1.94	0.67
1:A:276:ASN:ND2	1:A:365:MET:HE3	2.09	0.66
1:A:369:ARG:HD2	1:A:369:ARG:O	1.96	0.66
1:B:331:LYS:NZ	1:B:413:HIS:ND1	2.42	0.66
1:B:435:GLU:HG3	2:B:1442:WLM:C14	2.25	0.66
1:A:276:ASN:ND2	3:A:1443:1PE:C25	2.60	0.64
1:A:180:LYS:NZ	1:A:184:ASN:HD21	1.95	0.64
1:A:219:LEU:CD2	1:A:241:ILE:HD11	2.28	0.64
1:A:429:LEU:CB	1:A:434:GLN:HG2	2.27	0.64
1:A:269:SER:HB3	1:A:373:ILE:HD11	1.82	0.62
1:A:180:LYS:HZ1	1:A:184:ASN:HD21	1.49	0.61
3:A:1443:1PE:C22	1:B:236:PRO:HB3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:HIS:HA	1:A:416:MET:CE	2.30	0.61
1:B:420:ILE:HA	1:B:423:THR:HG22	1.82	0.61
1:A:367:VAL:N	1:A:368:PRO:HD2	2.16	0.61
1:B:250:GLN:HG2	1:B:433:LEU:HD12	1.83	0.60
1:B:317:LEU:HD21	2:B:1441:WLM:H5	1.83	0.60
1:A:357:LEU:CD2	1:A:373:ILE:HB	2.33	0.59
1:A:367:VAL:O	1:A:371:GLU:HG3	2.01	0.59
1:B:367:VAL:N	1:B:368:PRO:HD2	2.18	0.58
1:B:419:ARG:O	1:B:423:THR:HG22	2.03	0.58
1:A:192:MET:SD	1:A:196:LYS:HG2	2.44	0.58
1:A:269:SER:O	1:A:272:SER:HB2	2.02	0.58
1:B:367:VAL:HG22	1:B:368:PRO:HD3	1.84	0.57
1:A:219:LEU:HD23	1:A:241:ILE:CD1	2.34	0.57
1:B:219:LEU:O	1:B:223:GLU:HG3	2.05	0.57
1:A:192:MET:CE	1:A:196:LYS:HE2	2.35	0.56
1:A:276:ASN:ND2	3:A:1443:1PE:H252	2.20	0.56
1:A:192:MET:SD	1:A:196:LYS:HE2	2.45	0.56
1:A:429:LEU:HB3	1:A:434:GLN:CG	2.35	0.56
1:B:417:MET:HG3	1:B:437:TYR:CE2	2.40	0.56
1:A:438:LYS:HG2	1:A:439:ASP:N	2.19	0.56
1:B:192:MET:HE2	1:B:192:MET:HA	1.87	0.55
1:A:357:LEU:HD22	1:A:373:ILE:HG22	1.88	0.55
1:A:366:ASN:OD1	1:A:368:PRO:HG2	2.06	0.55
1:B:435:GLU:OE1	1:B:438:LYS:NZ	2.30	0.55
1:A:430:HIS:CE1	1:A:431:PRO:HD2	2.41	0.54
1:B:284:TYR:HB3	1:B:361:ARG:HD2	1.89	0.54
1:A:408:GLN:HA	1:A:408:GLN:NE2	2.21	0.54
1:A:357:LEU:HD22	1:A:373:ILE:CG2	2.37	0.54
1:A:343:LEU:HD11	1:A:399:LEU:HD21	1.90	0.54
1:B:219:LEU:HD23	1:B:241:ILE:HD11	1.90	0.53
1:B:268:PRO:O	1:B:269:SER:HB2	2.08	0.53
1:B:201:LEU:HG	1:B:304:LEU:HD11	1.90	0.53
1:A:276:ASN:HD21	3:A:1443:1PE:H252	1.74	0.53
1:B:357:LEU:CD2	1:B:373:ILE:HB	2.36	0.53
1:B:430:HIS:CG	1:B:431:PRO:HD2	2.43	0.53
1:A:248:ARG:CG	1:A:248:ARG:HH11	2.21	0.53
1:A:431:PRO:HG2	1:B:275:LEU:HG	1.89	0.53
1:B:429:LEU:HB2	1:B:434:GLN:HG3	1.91	0.52
1:A:419:ARG:O	1:A:423:THR:HB	2.10	0.52
1:A:435:GLU:OE1	1:B:435:GLU:OE2	2.27	0.52
1:B:423:THR:HG23	1:B:424:GLU:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:VAL:O	1:B:258:ARG:HG3	2.10	0.52
2:B:1441:WLM:O23	2:B:1441:WLM:S26	2.67	0.52
1:A:319:SER:OG	4:A:2039:HOH:O	2.19	0.51
1:A:329:GLU:N	1:A:330:PRO:HD2	2.26	0.51
1:B:288:GLU:HG3	1:B:410:VAL:HG21	1.92	0.51
1:B:214:HIS:HB2	4:B:2021:HOH:O	2.10	0.51
1:A:355:ILE:HG22	1:A:356:ILE:HD13	1.92	0.51
1:B:424:GLU:HG2	1:B:427:THR:CG2	2.41	0.50
1:B:248:ARG:CG	1:B:248:ARG:HH11	2.25	0.50
1:A:276:ASN:HB2	1:A:365:MET:HE1	1.92	0.50
1:A:274:PHE:CZ	3:A:1443:1PE:H121	2.47	0.50
1:A:402:LYS:HA	1:A:405:ASP:OD2	2.11	0.50
1:A:367:VAL:N	1:A:368:PRO:CD	2.75	0.49
1:A:396:PHE:HB3	1:A:397:PRO:HD3	1.94	0.49
1:A:365:MET:HE2	3:A:1443:1PE:H242	1.91	0.49
1:A:276:ASN:HD21	3:A:1443:1PE:C14	2.25	0.49
2:A:1442:WLM:O6	2:A:1442:WLM:N8	2.46	0.49
1:A:367:VAL:HG13	4:A:2052:HOH:O	2.10	0.49
1:B:219:LEU:CD2	1:B:241:ILE:HD11	2.42	0.49
1:A:235:LEU:HD23	1:A:251:CYS:SG	2.52	0.49
1:B:306:ALA:O	1:B:309:SER:OG	2.28	0.48
1:B:225:GLY:HA2	1:B:228:TRP:O	2.14	0.48
1:A:178:PHE:CE1	1:A:268:PRO:HG2	2.48	0.48
1:A:229:LYS:HB3	1:A:229:LYS:NZ	2.28	0.48
1:B:241:ILE:HG23	1:B:242:SER:N	2.29	0.47
1:A:217:GLU:O	1:A:221:GLN:HG3	2.14	0.47
1:B:235:LEU:HB3	1:B:236:PRO:HD2	1.96	0.47
1:B:178:PHE:HE1	1:B:268:PRO:HG2	1.75	0.47
1:A:248:ARG:CG	1:A:248:ARG:NH1	2.76	0.47
1:A:282:LEU:O	1:A:286:VAL:HG13	2.13	0.47
1:B:375:ASP:OD2	1:B:379:ARG:NH2	2.46	0.47
1:A:438:LYS:HG2	1:A:439:ASP:OD1	2.15	0.47
1:A:396:PHE:HB3	1:A:397:PRO:CD	2.45	0.46
1:A:276:ASN:HD21	3:A:1443:1PE:C25	2.26	0.46
1:B:430:HIS:CE1	1:B:432:LEU:HB3	2.51	0.46
1:A:276:ASN:ND2	3:A:1443:1PE:C14	2.78	0.46
1:A:429:LEU:HD11	1:A:437:TYR:CE2	2.50	0.46
1:B:198:ARG:HD3	1:B:198:ARG:HA	1.51	0.46
1:B:192:MET:HG2	1:B:297:ILE:HG21	1.97	0.46
1:B:424:GLU:HB3	1:B:427:THR:HG23	1.97	0.46
1:A:435:GLU:OE2	2:A:1442:WLM:H131	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ARG:NH1	1:B:248:ARG:HG2	2.30	0.46
1:B:367:VAL:N	1:B:368:PRO:CD	2.78	0.46
1:B:192:MET:CE	1:B:192:MET:HA	2.46	0.46
1:A:276:ASN:ND2	1:A:365:MET:CE	2.79	0.45
1:A:273:LEU:CD2	1:A:369:ARG:HG3	2.46	0.45
1:B:277:ASP:O	1:B:281:LEU:HG	2.17	0.45
1:B:396:PHE:N	1:B:397:PRO:HD2	2.31	0.45
1:A:358:CYS:SG	1:A:407:ARG:NH2	2.89	0.45
1:B:255:GLU:O	1:B:259:GLU:HG3	2.17	0.45
1:B:399:LEU:HD23	1:B:399:LEU:HA	1.83	0.45
1:A:424:GLU:HB3	1:A:427:THR:HG23	1.97	0.45
1:A:242:SER:OG	1:A:321:ARG:HB2	2.17	0.45
1:A:276:ASN:HD21	3:A:1443:1PE:H141	1.82	0.45
2:A:1441:WLM:S26	2:A:1441:WLM:O23	2.75	0.44
1:B:284:TYR:CB	1:B:361:ARG:HD2	2.46	0.44
1:B:396:PHE:HB3	1:B:397:PRO:HD3	1.99	0.44
2:B:1442:WLM:N8	2:B:1442:WLM:O6	2.50	0.44
1:B:423:THR:CG2	1:B:424:GLU:N	2.80	0.44
1:B:329:GLU:N	1:B:330:PRO:CD	2.80	0.44
1:A:275:LEU:HB3	3:A:1443:1PE:H251	1.98	0.44
1:A:429:LEU:HB2	1:A:434:GLN:HG2	1.98	0.44
1:A:421:LYS:HZ1	1:A:434:GLN:NE2	2.12	0.44
2:B:1442:WLM:S26	2:B:1442:WLM:O24	2.75	0.44
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.69	0.44
1:A:284:TYR:HB3	1:A:361:ARG:HD2	2.00	0.44
1:A:430:HIS:CG	1:A:431:PRO:CD	2.99	0.44
1:A:263:PHE:CE2	1:A:352:ILE:HG22	2.53	0.43
1:B:178:PHE:HE1	1:B:268:PRO:HB2	1.83	0.43
1:B:201:LEU:HD21	1:B:304:LEU:HG	2.00	0.43
1:B:258:ARG:NH2	4:B:2012:HOH:O	2.41	0.43
1:B:357:LEU:CD2	1:B:373:ILE:CG2	2.97	0.43
1:A:356:ILE:HG22	1:A:356:ILE:O	2.19	0.43
1:B:188:LYS:O	1:B:188:LYS:HG2	2.18	0.43
1:B:248:ARG:CG	1:B:248:ARG:NH1	2.81	0.42
1:B:250:GLN:HG2	1:B:433:LEU:CD1	2.49	0.42
1:B:314:ARG:HG2	1:B:318:ARG:HD2	2.01	0.42
1:A:220:TRP:NE1	1:A:224:LYS:HD2	2.35	0.42
1:A:298:VAL:HG22	1:A:303:LEU:HB3	2.02	0.42
1:B:430:HIS:ND1	1:B:431:PRO:HD2	2.35	0.42
1:B:211:PHE:CD2	1:B:222:ALA:HB2	2.54	0.42
1:B:407:ARG:HB2	1:B:407:ARG:HE	1.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:PHE:CE2	1:B:222:ALA:HB2	2.55	0.41
1:A:314:ARG:O	1:A:318:ARG:HG3	2.20	0.41
1:A:399:LEU:HA	1:A:399:LEU:HD23	1.70	0.41
1:A:429:LEU:CB	1:A:434:GLN:CG	2.98	0.41
1:A:235:LEU:CD2	1:A:251:CYS:SG	3.09	0.41
1:B:282:LEU:O	1:B:286:VAL:HG13	2.19	0.41
1:A:198:ARG:HA	1:A:198:ARG:HD3	1.74	0.41
1:B:364:LEU:HD23	1:B:364:LEU:HA	1.97	0.41
1:A:357:LEU:CD2	1:A:373:ILE:CG2	2.99	0.40
1:A:429:LEU:HD11	1:A:437:TYR:HE2	1.84	0.40
1:B:424:GLU:CG	1:B:427:THR:HG23	2.51	0.40
1:A:276:ASN:HD22	1:A:365:MET:HE3	1.82	0.40
1:B:298:VAL:HG22	1:B:303:LEU:HB3	2.03	0.40
1:A:430:HIS:ND1	1:A:431:PRO:CD	2.81	0.40
2:A:1442:WLM:H321	1:B:278:GLN:NE2	2.36	0.40
1:B:289:ALA:HB1	1:B:352:ILE:HG23	2.04	0.40
1:A:365:MET:HE3	3:A:1443:1PE:C24	2.40	0.40
1:B:224:LYS:C	1:B:226:LEU:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	257/288 (89%)	250 (97%)	7 (3%)	0	100	100
1	B	253/288 (88%)	237 (94%)	14 (6%)	2 (1%)	22	26
All	All	510/576 (88%)	487 (96%)	21 (4%)	2 (0%)	38	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	438	LYS
1	B	227	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/253 (92%)	206 (89%)	26 (11%)	7	7
1	B	228/253 (90%)	203 (89%)	25 (11%)	7	8
All	All	460/506 (91%)	409 (89%)	51 (11%)	7	8

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	ASP
1	A	195	LYS
1	A	198	ARG
1	A	223	GLU
1	A	230	GLN
1	A	248	ARG
1	A	250	GLN
1	A	269	SER
1	A	275	LEU
1	A	283	LYS
1	A	300	LYS
1	A	322	LYS
1	A	329	GLU
1	A	352	ILE
1	A	357	LEU
1	A	358	CYS
1	A	360	ASP
1	A	365	MET
1	A	403	MET
1	A	412	GLU
1	A	418	GLN
1	A	422	LYS

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Mol	Chain	Res	Type
1	A	423	THR
1	A	425	THR
1	A	426	GLU
1	A	427	THR
1	B	198	ARG
1	B	208	THR
1	B	226	LEU
1	B	228	TRP
1	B	248	ARG
1	B	250	GLN
1	B	255	GLU
1	B	300	LYS
1	B	315	GLU
1	B	318	ARG
1	B	322	LYS
1	B	328	ILE
1	B	331	LYS
1	B	360	ASP
1	B	365	MET
1	B	375	ASP
1	B	383	PHE
1	B	391	ASP
1	B	393	GLN
1	B	407	ARG
1	B	419	ARG
1	B	422	LYS
1	B	425	THR
1	B	426	GLU
1	B	427	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	191	ASN
1	A	230	GLN
1	A	276	ASN
1	A	384	HIS
1	A	388	ASN
1	A	401	GLN
1	A	408	GLN
1	A	415	GLN

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Mol	Chain	Res	Type
1	A	434	GLN
1	B	184	ASN
1	B	214	HIS
1	B	276	ASN
1	B	278	GLN
1	B	388	ASN
1	B	408	GLN
1	B	434	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	WLM	A	1441	-	32,34,34	1.57	2 (6%)	40,48,48	1.30	4 (10%)
2	WLM	A	1442	-	32,34,34	1.54	3 (9%)	40,48,48	1.58	3 (7%)
3	1PE	A	1443	-	15,15,15	0.36	0	14,14,14	0.59	0
2	WLM	B	1441	-	32,34,34	1.53	2 (6%)	40,48,48	1.25	3 (7%)
2	WLM	B	1442	-	32,34,34	1.67	4 (12%)	40,48,48	1.30	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WLM	A	1441	-	-	0/23/27/27	0/2/3/3
2	WLM	A	1442	-	-	0/23/27/27	0/2/3/3
3	1PE	A	1443	-	-	0/13/13/13	0/0/0/0
2	WLM	B	1441	-	-	0/23/27/27	0/2/3/3
2	WLM	B	1442	-	-	0/23/27/27	0/2/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1441	WLM	C28-N29	-4.27	1.28	1.33
2	B	1442	WLM	C28-N29	-3.97	1.28	1.33
2	B	1441	WLM	C28-N29	-3.74	1.29	1.33
2	A	1442	WLM	C28-N29	-3.36	1.29	1.33
2	B	1442	WLM	O6-C2	2.03	1.40	1.37
2	A	1442	WLM	O6-C2	2.07	1.40	1.37
2	B	1442	WLM	C28-C30	2.14	1.54	1.50
2	A	1441	WLM	S21-N22	6.22	1.74	1.63
2	A	1442	WLM	S21-N22	6.46	1.74	1.63
2	B	1441	WLM	S21-N22	6.46	1.74	1.63
2	B	1442	WLM	S21-N22	7.11	1.75	1.63

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1442	WLM	C25-N22-S21	-8.17	110.80	124.33
2	B	1442	WLM	C25-N22-S21	-5.86	114.64	124.33
2	A	1441	WLM	C25-N22-S21	-5.67	114.95	124.33
2	B	1441	WLM	C25-N22-S21	-5.54	115.16	124.33
2	A	1442	WLM	C2-C1-C4	-2.03	122.28	126.04
2	A	1441	WLM	O23-S21-C20	2.03	110.47	107.95
2	B	1441	WLM	O23-S21-C20	2.12	110.58	107.95
2	A	1441	WLM	C32-C30-C31	2.14	115.67	110.34
2	B	1441	WLM	C20-S21-N22	2.56	110.12	106.83
2	A	1442	WLM	O24-S21-C20	2.75	111.36	107.95
2	B	1442	WLM	C20-S21-N22	2.80	110.43	106.83
2	A	1441	WLM	C20-S21-N22	3.50	111.33	106.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1441	WLM	1	0
2	A	1442	WLM	6	0
3	A	1443	1PE	16	0
2	B	1441	WLM	2	0
2	B	1442	WLM	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	263/288 (91%)	0.09	8 (3%) 51 58	21, 36, 60, 83	0
1	B	259/288 (89%)	0.30	16 (6%) 21 28	27, 46, 73, 83	0
All	All	522/576 (90%)	0.19	24 (4%) 33 40	21, 42, 69, 83	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	383	PHE	5.7
1	B	202	THR	4.9
1	B	425	THR	3.7
1	A	383	PHE	3.7
1	B	208	THR	3.6
1	B	199	SER	3.4
1	B	322	LYS	3.2
1	B	177	ALA	3.1
1	A	234	GLY	3.0
1	B	210	PRO	2.9
1	A	230	GLN	2.9
1	B	201	LEU	2.8
1	B	391	ASP	2.8
1	A	440	MET	2.7
1	A	439	ASP	2.7
1	B	173	ALA	2.6
1	B	386	GLN	2.5
1	B	227	VAL	2.5
1	A	174	ASP	2.4
1	A	206	SER	2.3
1	B	175	LEU	2.2
1	B	212	VAL	2.1
1	B	174	ASP	2.1
1	A	208	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	1PE	A	1443	16/16	0.75	0.18	0.68	64,70,72,73	0
2	WLM	A	1441	32/32	0.96	0.13	0.57	20,28,41,52	0
2	WLM	B	1442	32/32	0.94	0.14	-0.10	35,44,73,75	0
2	WLM	A	1442	32/32	0.95	0.15	-0.10	37,57,79,80	0
2	WLM	B	1441	32/32	0.96	0.13	-0.40	26,37,55,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.